Synthesis and characterization of nitrile-functionalized pyridinium ionic liquids

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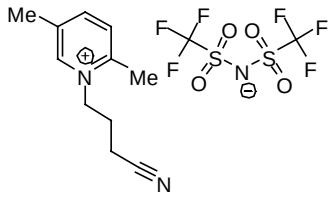
Nowadays functionalized ionic liquids with unique physiochemical properties are one of the major areas in ionic liquid research. Among them the nitrile- functionalized ionic liquids are of great importance because they find applications as reaction media and ligands for the catalytic reactions, electrolyte for lithium batteries and in dye-sensitized solar cells [1-2]. They are also relatively more stable than other types of functionalized ionic liquids. The nitrile ionic liquids can be considered as non-volatile analogues of acetonitrile. We synthesized and characterized a series of nitrile-functionalized pyridinium ionic liquids. We studied the physical properties of these ionic liquids by varying the substituents on the pyridine ring and altering the chain length of the alkyl group bearing the nitrile functionality. We also carried out a theoretical study of different cations of the nitrile-functionalized ionic liquids. In particularly, we calculated the natural partial charge (NPA) and the absolute isotropic shielding at nitrogen of the nitrile function (N_{CN}). For isolated molecule calculations, we find for similar cationic compounds an increased negative charge at N_{CN} with increasing spacer to the positive charged center of the cation. The same trend was observed for the 15N chemical shift in the NMR spectra of the nitrile-functionalized pyridinium ionic liquids. We also studied the electrochemical stability analysis of the nitrile-functionalized pyridinium ionic liquids



[1] Zhao DB, Fei ZF, Geldbach TJ, et al., *J. Am. Chem. Soc.* 126 (2004) 15876.
[2] Hardacre C, Holbrey JD, Mullan CL, et al., *New J. Chem.* 32 (2008) 1953.